

# EXHIBIT 1

# **APPLIED GROUNDWATER MODELING**

## Simulation of Flow and Advective Transport

**Second Edition**

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The front cover image is provided courtesy of Schlumberger Water Services. The image represents a uniform grid for a multi-layer finite-difference MODFLOW model and was produced using the software Visual MODFLOW Flex. Colors at the top of the image represent changes in land surface elevation; colors in the bottom layers represent geologic variability. The back cover graphic is a word cloud created using all text contained in Chapters 1–12. Word-cloud graphics included with the introductory sections of the book consist of text contained in each section. All word clouds were generated using Wordle, created by Jonathon Feinberg ([www.wordle.net](http://www.wordle.net)).

# CHAPTER 1

## Introduction

*Science, like art, is not a copy of nature but a re-creation of her.*

*Jacob Bronowski (1956, Science and Human Values Part 1)*

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## 1.1 MOTIVATION FOR MODELING

Groundwater hydrologists are often asked questions about groundwater flow systems and management of groundwater resources. The following is a representative sampling of these types of questions.

*How will pumping affect groundwater levels in the North China Plain in the next 100 years?  
How will proposed land use change affect groundwater discharge to wetlands and streams in  
Madison, Wisconsin, USA?*

*How will water management decisions related to water diversions affect groundwater levels in the  
Nubian Sandstone of Egypt and Libya in the next 50 years?*

*How will climate change affect groundwater levels and groundwater discharge to surface water  
bodies in temperate forests in northern Wisconsin, USA?*

*How long will it take for water levels in a lake created as a result of open pit mining in Guyana to  
reach equilibrium after dewatering operations cease?*

*What is the capture area of a well field that supplies municipal water to Graz, Austria?*

*Where and when should groundwater be sampled to identify potential leakage of a clay liner  
beneath a landfill in Mexico City?*

*How long will it take contaminants leaching into groundwater from an abandoned industrial site  
in Tokyo to reach the property boundary?*

Providing answers to these seemingly straightforward questions requires considerable specific hydrogeologic information and analyses, as well as general hydrogeologic knowledge, insight, and professional judgment. Even relatively simple groundwater problems require values of aquifer parameters and hydrologic stresses such as pumping and recharge rates.

A groundwater model provides a quantitative framework for synthesizing field information and for conceptualizing hydrogeologic processes. The organization imposed by a model helps alert the modeler to errors in assumptions and to processes not previously considered. In other words: "...applying a model is an exercise in thinking about the way a system works" (Anderson, 1983). For this reason, mathematical modeling should be performed at the beginning of every hydrogeological study that addresses nontrivial questions (e.g., see Bredehoeft and Hall, 1995).

Tóth (1963) gave compelling justification for modeling, which is still valid today: "Whereas it is practically impossible to observe separately all phenomena connected with a regime of groundwater flow, a correct theory discloses every feature and draws attention to the most important properties of the flow." Or put another way, given that the subsurface is hidden from view and analysis is hampered by lack of field observations, a model is the most defensible description of a groundwater system for informed and quantitative analyses as well as forecasts about the consequences of proposed actions.

Therefore, although not all hydrogeological problems require a model, almost every groundwater problem will benefit from some type of model, if only as a way to organize field data and test the conceptual model. A corollary to the question "why model?" is the question "what else if not a model?" In the 1st edition of this book we included discussion of the debate over the worth of models then current in the literature. Today, groundwater models are accepted as essential tools for addressing groundwater problems.

## 1.2 WHAT IS A MODEL?

A *model* is a simplified representation of the complex natural world. For example, a road map is a kind of model (Wang and Anderson, 1982); it depicts a complex network of roads in a simplified manner for purposes of navigation. Similarly, a conceptual model of a groundwater system simplifies and summarizes what is known about the hydrogeology in the form of written text, flow charts, cross sections, block diagrams, and tables. A conceptual model is an expression of the past and current state of the system based on field information from the site, and knowledge available from similar sites (Section 2.2). A more powerful groundwater model is one that quantitatively represents heads in space and time in a simplified representation of the complex hydrogeologic conditions in the subsurface. Broadly speaking, groundwater models can be divided into physical (laboratory) models and mathematical models.

### 1.2.1 Physical Models

Physical models include laboratory tanks and columns packed with porous material (usually sand) in which groundwater heads and flows are measured directly. For example, in pioneering work Darcy (1856) measured head in sand-packed columns of various diameters and lengths to show that flow in porous media is linearly related to the head gradient. Physical models are mostly used at the laboratory scale (e.g., Mamer and Lowry, 2013; Illman et al., 2012; Sawyer et al., 2012; Fujinawa et al., 2009). Analog models are laboratory models that rely on the flow of electric current (electric analog models; e.g., Skibitzke, 1961) or viscous fluids (Hele-Shaw or parallel plate models; e.g., Collins and Gelhar, 1971) to represent groundwater flow. Analog models of groundwater flow, especially electric analog models, were important in the 1960s before digital computers were widely available (e.g., see Bredehoeft, 2012).

### 1.2.2 Mathematical Models

We consider two types of mathematical models: data-driven models and process-based models. *Data-driven or “black-box” models* (Box 1.1) use empirical or statistical equations derived from the available data to calculate an unknown variable (e.g., head at the water table) from information about another variable that can be measured easily (e.g., precipitation). *Process-based models* (sometimes called physically based models although that usage is discouraged by Beven and Young, 2013) use processes and principles of physics to represent groundwater flow within the problem domain. Process-based models are either stochastic or deterministic. A model is *stochastic* if any of its parameters have a probabilistic distribution; otherwise, the model is *deterministic*. The focus of our book is process-based deterministic models, although we briefly discuss stochastic models in Boxes 10.1 and 10.4 and Section 12.5.

A process-based mathematical groundwater flow model consists of a *governing equation* that describes the physical processes within the problem domain; *boundary conditions* that specify heads or flows along the boundaries of the problem domain; and for time-dependent problems, *initial conditions* that specify heads within the problem domain at the beginning of the simulation. Mathematical models can be solved analytically or numerically. Mathematical models for groundwater flow are solved for the distribution of head in space and also in time for transient problems.

Analytical models require a high level of simplification of the natural world in order to define a problem that can be solved mathematically to obtain a closed-form solution. The resulting analytical solution is an equation that solves for a dependent variable (e.g., head) in space and for transient problems also in time. Simple analytical solutions can be solved using a hand calculator but more complex solutions are often solved using a spreadsheet or a computer program (e.g., Barlow and Moench, 1998), or special software (e.g., MATLAB, <http://www.mathworks.com/products/matlab/>). Assumptions built into analytical solutions limit their application to relatively simple systems and hence they are inappropriate for most practical groundwater problems. For example, few analytical solutions allow for three-dimensional flow or hydrogeological settings with heterogeneity or boundaries with realistic geometries. Numerical models are even replacing the Theis (1935) analytical solution for aquifer test analysis (e.g., Li and Neuman, 2007; Yeh et al., 2014). Nevertheless, analytical solutions are still useful for some problems

### Box 1.1 Data-Driven (Black-Box) Models

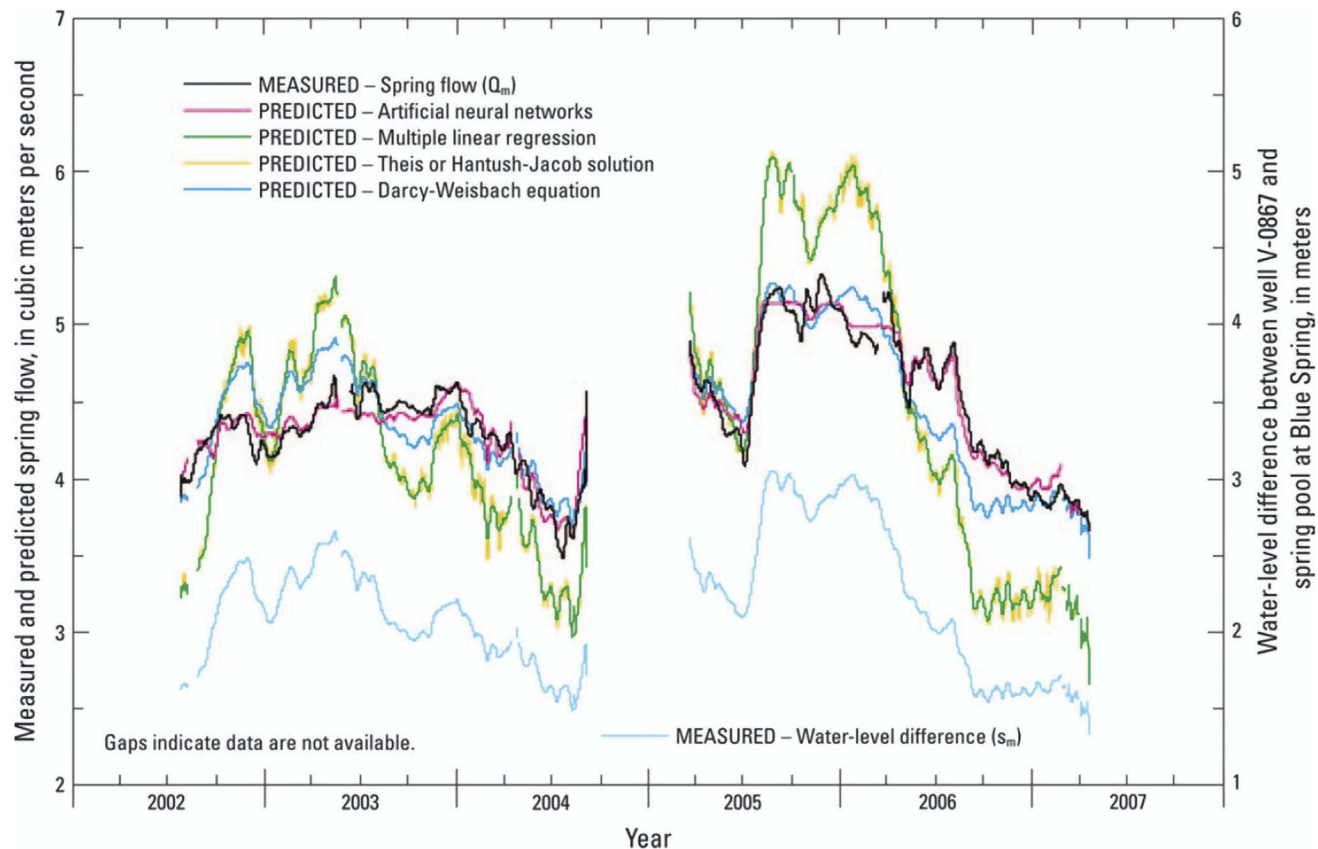
Data-driven models use equations that calculate system response (e.g., head) to input stresses (e.g., recharge from precipitation) without quantifying the processes and physical properties of the system. First, a site-specific equation is developed by fitting parameters either empirically or statistically to reproduce the historical record (time series) of fluctuations in water levels (or flows) in response to stresses. Then, the equation is used to calculate the response to future stresses. Data-driven models require a large number of observations of head that ideally encompass the range of all expected stresses to the system. They are used by themselves (e.g., Bakker et al., 2007) or with a process-based model (e.g., Gusyev et al., 2013; Demissie et al., 2009; Szidarovszky et al., 2007).

Early applications of data-driven models analyzed the response of karst aquifers (Dreiss, 1989) and applications to karst systems continue to be popular and successful (Fig. B1.1.1). Artificial neural network (ANN) models are data-driven models that have received much interest in the recent literature (e.g., Sepúlveda, 2009; Feng et al., 2008; Coppola et al., 2005). Data-driven models are also developed using Bayesian networks (e.g., Fienen et al., 2013).

Generally, process-based models are preferred over data-driven models because process-based models can make acceptable forecasts when large numbers of observations are not available and when future conditions lie outside the range of stresses in the historical record, such as response to climate change.



# Box 1.1—cont'd



**Figure B1.1.1** Springflow calculated using an ANN model and multiple linear regression compared with results from process-based models for continuous porous media (Theis or Hantush–Jacob solutions) and conduit flow (Darcy–Weisbach equation). Measured springflow is also shown (*Sepúlveda, 2009*).



and also provide important insight into the behavior of groundwater systems (Box 3.2). Analytical models can be useful interpretive tools to guide construction of more complex numerical models (Haitjema, 2006). Analytical solutions are also used to verify that codes that solve numerical models are programmed correctly (Section 1.6).

The analytic element (AE) method (Haitjema, 1995; Strack, 1989) provides a way to extend analytical solutions to more complex problems. The AE method relies on a computer code to superpose certain types of analytical solutions, known as analytic elements, which are based on Green's functions and include solutions with point/line sources and sinks. AE models can incorporate complex boundary geometry and zones of heterogeneity, but currently have limited applicability for highly heterogeneous and transient problems (Hunt, 2006), although development of new AE solutions is an active area of research (e.g., Kulman and Neuman, 2009). Currently, AE models are most commonly applied to two-dimensional and steady-state groundwater flow problems (e.g., see Hunt, 2006; Haitjema, 1995). AE models are also useful for guiding assignment of regional boundary conditions for three-dimensional and transient modeling (Section 4.4).

Numerical models, typically based on either the finite-difference (FD) or the finite-element (FE) method, allow for both steady-state and transient groundwater flow in three dimensions in heterogeneous media with complex boundaries and a complex network of sources and sinks. Owing to their versatility, FD and FE models are most commonly used to solve groundwater problems and are the focus of our book.

Mathematical groundwater models are used to simulate both local and regional settings. Although some questions can, and should, be addressed with analytical models or simple numerical models, many problems require a more sophisticated representation of the groundwater system. Increased computing power and new codes and tools allow complex and large regional systems to be efficiently simulated. The sophistication, or complexity, of a numerical model is often measured by the number of processes included and the number of layers, cells/elements, and parameters it contains. Numerical methods assign parameter values to points (nodes) in the model domain and it is not uncommon for models to have millions of nodes. For example, Frind et al. (2002) described a three-dimensional, 30-layer FE model of the Waterloo Moraine aquifer system (Ontario, Canada) that used 1,335,790 nodes and 2,568,900 elements. A three-dimensional FD model of the Lake Michigan Basin (Feinstein et al., 2010) used over two million nodes. Kollet et al. (2010) discussed groundwater models that contained  $8 \times 10^9$  FD cells. Although values of hydrogeologic parameters must be assigned to every node, cell, or element, in practice it is usual to delineate areas (zones) in the problem domain in which a constant value is assigned to all the nodes (Section 5.5). Hence, zonation effectively reduces the number of parameters. Other methods of parameterization and the issue of complexity in groundwater models are discussed in Chapter 9.

We use the term *groundwater model* or *model* to mean the mathematical representation and associated input data for a specific problem. A *code* is a computer program that

processes the input data for a specific model and solves the process-based equations (Section 3.2) that describe groundwater processes. A code is written in one or more computer languages and consists of a set of equations that is solved by a computer. For example, PEST and the FD code MODFLOW are written in the computer language Fortran; PEST++ and the FE code FEFLOW are written in C/C++. A code that solves for groundwater flow calculates head in space and time, along with associated quantities such as flow. A *particle tracking code* takes output from a groundwater flow code and calculates groundwater flowpaths and associated travel times (Chapter 8). Codes are sometimes called groundwater models but we distinguish between a specific application of a code, which is a model, and the code itself, which is the tool for solving the model. A different groundwater model is designed for each application whereas the same code is used to solve many different problems.

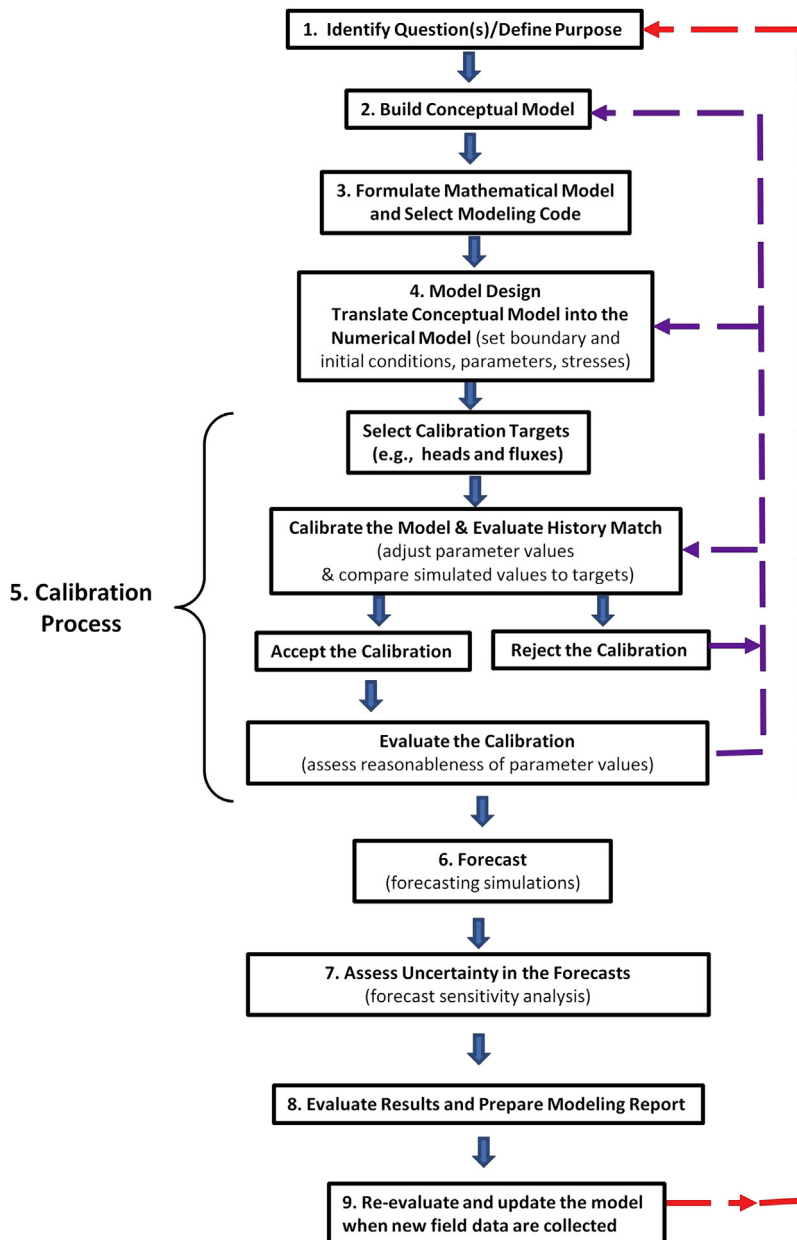
### 1.3 PURPOSE OF MODELING

The starting point of every groundwater modeling application is to identify the purpose of the model (Fig. 1.1). The most common purpose is to forecast the effects of some future action or hydrologic condition, but models are also used to re-create past conditions (hindcasting) and also as interpretive tools. Reilly and Harbaugh (2004, p. 3) identify five broad categories of problems for groundwater modeling: basic understanding of groundwater systems; estimation of aquifer properties; understanding the present; understanding the past; and forecasting the future. We group the first three of these categories into interpretive models and the last two into forecasting/hindcasting models. We discuss forecasting/hindcasting models first.

#### 1.3.1 Forecasting/Hindcasting Models

The objective of the vast majority of groundwater models is to forecast or predict results of a proposed action/inaction. Forecasting simulations are designed to address questions like those listed at the beginning of this chapter. We prefer the term forecast over prediction to emphasize that a forecast always contains some uncertainty. For example, a weather forecast is typically stated in terms of a probability (of rain, for example). Forecasting models (Chapter 10) are typically first tested by comparing model results to field measurements in a history matching exercise that is part of model calibration (Chapter 9). In history matching, parameters are adjusted within acceptable limits until model outputs, primarily heads and flows, give a satisfactory match to field-measured (observed) values. The calibrated model is then used as the base model for forecasting simulations.

*Hindcasting (or back-casting) models* are used to re-create past conditions. Hindcasting models may involve both a groundwater flow model and a contaminant transport model to simulate the movement of a contaminant plume. Examples of hindcasting models include those used in the well-known Woburn, Massachusetts Trial (Bair, 2001) and



**Figure 1.1** Workflow for groundwater modeling. As presented, the workflow assumes the objective of the model is a forecast but the workflow can be adapted for other modeling purposes, as described in the text. Although not shown in the figure, field data are critical for the workflow, especially conceptual model design and the calibration process.

at a military base in North Carolina (Clement, 2011). Hindcasting applications are “uniquely challenging” (Clement, 2011) because it is not possible to collect additional observations to augment the existing historical dataset, which is often meager.

### 1.3.2 Interpretative Models

Interpretive models include those used as: (1) *engineering calculators* that quickly give an answer to a specific engineering question; (2) *screening models* that help the modeler develop an initial understanding of a groundwater system and/or test hypotheses about the system; (3) *generic models* that explore processes in generic hydrogeologic settings. Models used as engineering calculators and generic models usually are not calibrated. Screening models may or may not be calibrated.

An example application of an interpretive model as an engineering calculator is the use of analytical and numerical models to calculate aquifer parameters from drawdown data obtained in an aquifer (pumping) test. Analytical models and sometimes numerical models are used as engineering calculators to verify new codes (Section 1.6).

A screening model vets a conceptual model or tests hypotheses about the flow system. A screening model might help in designing a more complex numerical model. For example, Hunt et al. (1998) developed a two-dimensional AE model as a screening model to develop boundary conditions for a three-dimensional FD model. Interpretive models also are used to conceptualize system dynamics and provide general insights into controlling parameters or processes at a field site. For example, during a major oil spill from a damaged well in the Gulf of Mexico, Hsieh (2011) quickly developed an interpretive MODFLOW model (adapted to simulate flow in a petroleum reservoir) to determine if measured shut-in pressure in the damaged well was indicative of a potential future catastrophic rupture of the capped well. The results were used to make the decision not to uncup the well to reduce reservoir pressure, which proved to be the correct course of action.

Generic models are interpretive models applied to idealized groundwater systems. Generic models were used in the early days of numerical modeling of groundwater flow and continue to be useful. For example, Freeze and Witherspoon (1967) and Zlotnik et al. (2011) used two-dimensional generic models to study the effects of heterogeneity on regional groundwater flow in cross section. Woessner (2000) and Sawyer et al. (2012) used generic models to study exchange between groundwater and streams at the aquifer/stream interface (the hyporheic zone). Sheets et al. (2005) used generic models to assess the effect of pumping near regional groundwater divides.

## 1.4 LIMITATIONS OF MODELS

Groundwater models are simplifications of reality and thus are limited by underlying simplifying approximations as well as by nonuniqueness and uncertainty (Chapters 9

and 10). Groundwater models never uniquely represent the complexity of the natural world. Therefore, groundwater models that represent the natural world have some level of uncertainty that must be evaluated and reported. In that respect, forecasting simulations for groundwater are similar to weather forecasts. Weather forecasts combine extensive datasets, representations of atmospheric physics, meteorology, and real-time satellite images within a highly sophisticated model, but the daily forecast is always given with probabilities. Similarly, results from groundwater models should be qualified by specifying the nature and magnitude of uncertainty associated with a forecast (Section 10.6).

### 1.4.1 Nonuniqueness

Nonuniqueness in groundwater models means that many different combinations of model inputs produce results that match field-measured data. Consequently, there will always be more than one possible reasonable model. Although early groundwater modeling applications typically reported only one calibrated model and presented only one possible forecast, this is unacceptable practice today. Either multiple calibrated models are carried forward in the analysis or the modeler chooses a preferred calibrated model and constructs error bounds around forecasted outputs. In either case, it is acknowledged that a groundwater model cannot give a single true answer.

Although models are critical tools, professional judgment, guided by modeling intuition and hydrogeological principles, is always required during a modeling project. Recognition of model uncertainty and nonuniqueness motivates the following underlying philosophy of modeling: "...a model cannot promise the right answer. However, if properly constructed, a model can promise that the right answer lies within the uncertainty limits which are its responsibility to construct" (Doherty, 2011).

### 1.4.2 Uncertainty

Uncertainty in groundwater models (Sections 10.2, 10.3) arises from a number of factors related to representing groundwater processes. In selecting a particular code, the modeler indirectly makes assumptions about the set of hydrologic processes important to the modeling objective because the selection of a code in effect reduces all processes under consideration to only those included in the code. Furthermore, current and future hydrogeologic conditions represented in a model cannot be fully described or quantified. Hunt and Welter (2010) described one source of uncertainty as "unknown unknowns," which are "...things we do not know we don't know" (from Former US. Secretary of Defense Donald Rumsfeld, February 12, 2002 press briefing). In groundwater models, *unknown unknowns* include unexpected (and hence unmodeled) hydrogeologic features such as heterogeneities in subsurface properties, as well as unanticipated future stresses. Bredehoeft (2005) cautioned modelers to anticipate the model "surprise" that occurs when new data reveal system responses caused by unmodeled hydrologic processes. For example, in a forecasting model there is uncertainty over future hydrological

conditions (e.g., recharge rates) as well as future pumping rates and locations of new wells, which depend on uncertain societal and economic drivers.

Although some types of forecasts are more uncertain than others (Section 10.3), uncertainty can only be reduced, never eliminated. Therefore, groundwater modelers need to develop an awareness of the uncertainties that influence modeling results and a healthy skepticism of modeling output. Modeling intuition (Haitjema, 2006) and “hydrosense” (Hunt and Zheng, 2012) help a modeler evaluate modeling output and identify flawed results. Modeling processes and results need to undergo rigorous “sensitivity analyses” that are rooted in basic hydrogeologic principles.

## 1.5 MODELING ETHICS

Ethics refer to pursuing a course of action that leads to morally right outcomes. Ethics in groundwater modeling means that the groundwater modeler acts in a morally responsible manner when planning, designing, and executing models and presenting modeling results. Ethics also means that the modeler remains unbiased and objective and strives to model according to the best available science for the modeling purpose. The modeler must maintain scientific integrity even when the results are not what the client expects, and when models enter regulatory and legal arenas. Tensions can arise between the modeler and teams of interdisciplinary scientists, lawyers, regulators, and stakeholders including industrial clients and the public-at-large. The modeler must resist inappropriate pressure from those groups as well as the pressure of societal, environmental, and regulatory concerns and steadfastly perform ethical modeling.

Modeling may be driven by regulatory concerns or even mandated by regulations. For example, groundwater models are required by the European Water Framework Directive (Hulme et al., 2002) or regulations may be written in such a way that the best (perhaps even only) way to satisfy a regulatory obligation is by groundwater modeling. When models are discussed in the courtroom, the modeler must be especially vigilant to present objective, unbiased results based on sound science. The U.S. Federal Court trial regarding groundwater contamination in Woburn, Massachusetts, which was the subject of a popular book (Harr, 1995) and a movie (*A Civil Action*), was notable for the conflict and confusion that surrounded the interpretation of the hydrogeologic system (Bair, 2001; Bair and Metheny, 2011; also see *Science in the Courtroom: The Woburn Toxic Trial*: <http://serc.carleton.edu/woburn/index.html>). In that case, competing groundwater models (a one-dimensional steady-state model and a three-dimensional, transient model) and differences in opinion among three expert witnesses over the basic hydrogeology and appropriate parameter values led to difficulties in fact-finding needed to reach a verdict.

Ethical issues may arise over decisions about model design (especially as related to model complexity), model bias, presentation of results, and costs of modeling. Each of these is discussed below.

### 1.5.1 Model Design

In designing a model, the groundwater hydrologist, sometimes in concert with the client, regulators and stakeholders, proposes the analyses best suited to address the question(s) being posed. A numerical groundwater model may not be necessary if the questions can be answered more effectively using an analytical solution, an AE model, a data-driven model (Box 1.1), or analysis of field data without a model. For example, Kelson et al. (2002) showed that a simple AE model quickly provided the same insight into the effects of dewatering caused by a proposed mine as complex three-dimensional numerical models. However, for many complex problems a numerical model may be the best way to answer the questions. For the mine site considered by Kelson et al. (2002), questions about on-site disposal of mine tailings and the potential for contamination of groundwater and surface water were best addressed with a more comprehensive numerical model.

It may be clear before, during, or after a modeling effort that the available data are inadequate to constrain modeling results to a reasonable range suitable for decision-making. Clement (2011) discussed a highly complex state-of-the-art numerical hindcasting model where the historical data were judged insufficient to support the modeling effort. An independent panel of experts recommended that future hindcasting models for other parts of the site utilize simpler models including analytical models. The modelers disagreed with that assessment (Maslia et al., 2012), arguing that complex models are useful even when not fully supported by field data. The argument over simplicity *vs* complexity when designing groundwater models is a common topic in the literature (e.g., Simmons and Hunt, 2012; Hunt et al., 2007; Hill, 2006; Gómez-Hernández, 2006). Models should include processes and parameters essential to addressing the model's purpose, but exclude those that are not. Defining the optimal compromise between simplicity and complexity is part of the art of modeling and is one of the biggest challenges in modeling (Doherty, 2011). Simplifications come in many forms—for example, in the processes included or excluded from the model, and in the discretization of space and time, selection of boundary conditions, and parameter assignment. Each decision to simplify the complex natural world will influence the model's ability to simulate some facet of the actual hydrogeologic conditions.

### 1.5.2 Bias

Critics of modeling argue that models can be designed to produce whatever answer the modeler wants. Professionalism and ethics, however, require the modeler to design the model without introducing approximations that bias results. A simple example of deliberate bias is if a modeler consciously and inappropriately assigns a specified head boundary condition in order to minimize drawdown from pumping. (A specified head boundary allows an infinite amount of water to flow into the model and thereby mitigates the effect



of pumping by maintaining heads at unnaturally high levels (Section 4.3).) Concerns over bias motivate a requirement for peer review of modeling reports (Section 11.4). In-house review by senior hydrogeologists or engineers and by outside experts, regulators, opposing parties, and even the interested public is common. Quality assurance review can be helpful to the modeler in identifying inadvertent modeling errors, but when performed by an independent party, especially one engaged by an opposing party, such errors can support concerns of deliberate bias. The perception of bias is reinforced if either the modeler or reviewers neglect to reveal any potential conflicts of interest and areas of personal bias.

Critics often question whether a modeler paid by a client can remain independent and avoid bias. It is essential that modelers maintain their independence and preserve their professional credibility. The modeler has the obligation to give honest scientific and engineering assessments in return for compensation for work performed. The payment for work performed is not itself at issue but there may be the perception that the resulting model is biased to produce results favorable to the client. Such concerns over perceived bias can be addressed by careful and deliberate presentation of results, as discussed below.

### 1.5.3 Presentation of Results

With today's sophisticated codes and graphics packages it is relatively easy to produce visually impressive figures and tables. But ethics require that assumptions and approximations built into the model are clearly identified in the modeling report and in oral presentations. Inadequacies in field data should be discussed and uncertainties in modeling results should be quantified and discussed. Directly addressing potential concerns about the model's trustworthiness helps safeguard the modeler against claims of bias. Preparation of the modeling report is discussed in Chapter 11.

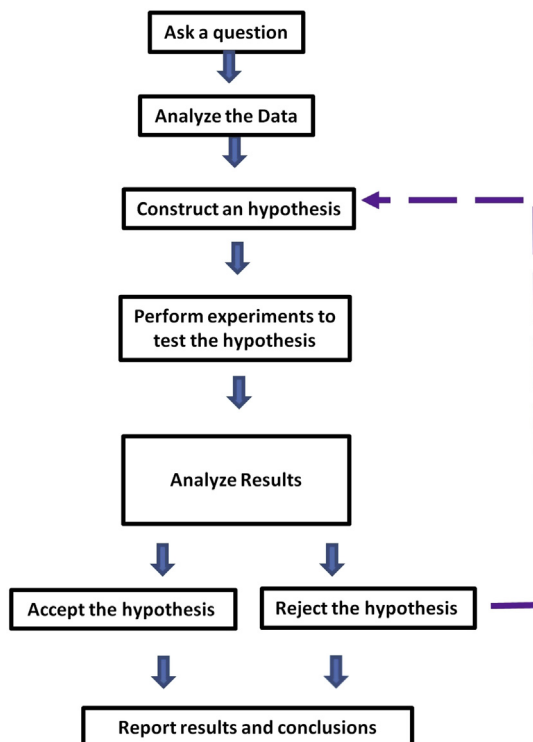
### 1.5.4 Cost

The cost of designing and executing a numerical model is sometimes cited as a limitation of modeling, but we consider it an ethical concern. After an investment in hardware and software, the costs of modeling are primarily for the modeler's and modeling team's time. Obviously, a complicated model requires more time and money to construct than a simple model. Missteps in conceptualization, construction, execution, and interpretation of models cost time and money but are often an unavoidable part of the modeling process. Of course, models need field data, but field data are needed for any type of hydrogeologic analysis. Availability of funds may limit the type of model that can be constructed and the scope of the modeling effort; the modeler is ethically bound to provide the best possible model given the time and resources available. When cost is the dominant driver for the model presented, the report should clearly state how constraints on funding affected the design of the model and the output.

## 1.6 MODELING WORKFLOW

Steps in groundwater modeling (Fig. 1.1) follow the scientific method (Fig. 1.2). In the scientific method, a question is asked, a hypothesis is constructed and tested, then accepted or rejected. If rejected, the testing process is repeated with a revised hypothesis. Similarly, the workflow for groundwater modeling starts with a question. Modeling should never be an end in itself; a model is always designed to answer a specific question or set of questions. The question underpins all facets of the resulting groundwater model. A workflow for applying groundwater models in forecasting is presented in Fig. 1.1. The steps in the workflow build confidence in the model. Although not shown in the figure, field data and soft knowledge (i.e., any information that is not evaluated directly by model output) inform almost every step of the modeling process, especially the design of the conceptual model, parameterization, selection of calibration targets, and ending the calibration process.

The modeling process may start over when new field data become available and when there are new questions to answer. The cyclic nature of the workflow allows for the



**Figure 1.2** The scientific method (modified from: [http://www.sciencebuddies.org/science-fair-projects/project\\_scientific\\_method.shtml](http://www.sciencebuddies.org/science-fair-projects/project_scientific_method.shtml)).

potential to improve and update the model when a calibrated groundwater model is used routinely as a decision-making tool in water resources management. Modelers in the UK are working toward establishing a set of calibrated models for aquifer systems throughout the UK for water resources management (Shepley et al., 2012). The Netherlands has a countrywide AE groundwater model (De Lange, 2006) and multimodel system for water resources management (De Lange et al., 2014); large regional models designed for water resources management are also being developed in the US (Reeves, 2010). More often, however, a model is developed to answer a specific question and after the decision is made, the model is rarely used again.

### 1.6.1 Steps in the Workflow

Our book is structured to discuss each of the steps in Fig. 1.1 as summarized below.

1. The purpose of the model (Chapter 2) is to answer a specific question or set of questions. The purpose is the primary factor in deciding appropriate simplifications and assumptions and thereby determines the characteristics of the mathematical model and drives code selection and model design.
2. The conceptual model (Chapter 2) consists of a description of the groundwater flow system including associated surface water bodies, as well as hydrostratigraphic units and system boundaries. Field data are assembled and the hydrogeologic system is described; water budget components are estimated. Multiple conceptual models may be constructed in order to account for uncertainty in describing the field setting. If the modeler did not collect the field data, a visit to the field site is recommended. A field visit will help put the hydrogeologic setting in perspective, give context to the assignment of parameter values and guide decisions during the modeling process.
3. The modeling purpose and the conceptual model drive the choice of a mathematical model and associated code(s) (Chapter 3). The mathematical model consists of a governing equation, boundary conditions, and, for transient problems, initial conditions. Numerical methods programmed into the code approximate the mathematical model.
4. Model design (Chapters 4–7) involves translating the conceptual model into a numerical groundwater flow model by designing the grid/mesh, setting boundaries, assigning values of aquifer parameters, and hydrologic stresses, and, for transient models, setting initial conditions and selecting time steps. The model is run using an initial set of parameter values (Section 5.5) based on the conceptual model. A particle tracking code (Chapter 8) is used to check flow directions and interactions with boundary conditions, and calculate flowpaths and travel times.
5. Arguably calibration (Chapter 9) is the most important step in the modeling process because it helps establish the legitimacy of the conceptual and numerical models. Moreover, the calibrated model is the base model for forecasting simulations. During

the calibration process, the modeler selects calibration targets and calibration parameters, and performs history matching. History matching consists of adjusting the initial parameter assignments in sequential model runs until field observations are sufficiently matched by the model and final parameter values are reasonable. A parameter estimation code helps find the values of calibration parameters that give the best possible match to the field observations (calibration targets). Modelers often do not allow sufficient time for calibration; a guideline is to start calibration no later than halfway (defined by the timeline and budget) through the project and preferably earlier.

6. Forecasting simulations (Chapter 10) use the calibrated model or a set of acceptably calibrated models to forecast the response of the system to future events; or the calibrated model is used to reconstruct past conditions in a hindcasting simulation. In both forecasts and hindcasts, the model is run using calibrated values for aquifer parameters and stresses except for stresses that change under future (or past) conditions. Estimates of anticipated future hydrologic conditions (e.g., recharge rates and pumping rates) are needed to perform the forecast; past hydrologic conditions are needed in hindcasts.
7. Uncertainty (Chapter 10) in a forecast (or hindcast) arises from uncertainty in the calibrated model, including its parameters, as well as uncertainty in the magnitude and timing of future (or past) hydrologic conditions. A forecasting uncertainty analysis includes assessment of measurement error, errors in the design of the model, and uncertainty in future (or past) hydrologic conditions important to the forecast (or hindcast). A particle tracking code may be used to forecast flowpaths and travel times (Chapter 8).
8. The results are presented in the modeling report and stored in the modeling archive (Chapter 11). The modeling report chronicles the modeling process, presents model results and states conclusions and limitations. It includes introductory material, information on the hydrogeologic setting, explanation of the data and assumptions used to formulate the conceptual model, and a reference to the numerical methods and code selected. The report also describes how the model domain is discretized and how parameters were assigned, documents model calibration and presents calibration results, forecasts and associated uncertainty. Modeling reports are accompanied by an archive that contains datasets, codes, input and output files and other materials needed to re-create and execute the model in the future.
9. When the opportunity arises it is useful to evaluate model performance by performing a postaudit. A *postaudit* (Section 10.7) compares the forecast with the response that actually occurred in the field as a result of the action that was simulated by the model. The postaudit is performed long enough after the forecast to allow adequate time for significant changes to occur in the field system. New field data collected during a postaudit may be used to improve the model. In *adaptive management* the model is routinely updated as new data become available and used to guide management decisions.

A forecasting simulation proceeds through steps 1 through 8. Engineering calculators and generic models require steps 1 through 4 and then skip to step 6. The steps in the workflow for a screening model depend on the purpose; the workflow always includes the first four steps and might proceed through step 5 or even steps 6, 7, and 8. If multiple possible conceptual models are considered (e.g., [Neuman and Wierenga, 2002](#)), the workflow is executed multiple times.

### 1.6.2 Verification and Validation

The terms model verification, code verification, and model validation are not in the workflow because verification and validation, as historically used, are no longer critical elements in groundwater modeling. However, because these terms are still in use, we discuss them below and also in Box 9.5.

*Model verification* refers to a demonstration that the calibrated model matches a set of field data independent of the data used to calibrate the model. However, given the large number of parameters involved in calibrating most field-based groundwater models, it is advisable to use all available data in the calibration exercise itself ([Doherty and Hunt, 2010](#), p. 15) rather than save some data for verification. Thus, groundwater model verification per se generally is not a useful exercise.

*Code verification* refers to a demonstration that a code can reproduce results from one or more analytical solutions or match a solution from a verified numerical code. Code verification is an important step in developing a code ([ASTM, 2008](#)) and information on code verification should be included in the user's manual. However, given that most applied modeling makes use of standard codes that have been verified by the code developer and well tested by the modeling community, additional code verification is not required for most modeling projects. Rather, it is reserved for cases when a new code is developed specifically for the modeling project or when an existing code is modified.

The term model validation has been much debated in the groundwater literature (e.g., [Konikow and Bredehoeft, 1992](#); associated comments and reply; [Bredehoeft and Konikow, 1993, 2012](#); [Anderson and Bates, 2001](#); [Hassan, 2004a,b](#); [Moriassi et al., 2012](#)). Validation has been equated with model calibration to suggest, incorrectly, that a calibrated model is a validated model. Furthermore, the term validation may incorrectly imply to nonmodelers that a model is capable of making absolutely accurate forecasts. This is fundamentally not supportable—truth cannot be demonstrated in any model of the natural world, or in any forecast using that model, because the truth is unknown ([Oreskes et al., 1994](#)). Therefore, models of the natural world cannot be validated in the same way as a computer code is verified or as a controlled laboratory experiment might be validated. Although such philosophical subtleties are not universally accepted, most groundwater modelers concur that a groundwater model cannot make absolutely

accurate forecasts and therefore cannot be validated. We recommend the term “validation” not be used in reference to a groundwater model.

The modeling workflow described above provides a generic structure for best modeling practice. Modeling guidelines also provide strategies for modeling but are formulated as required or recommended steps tailored to application in a regulatory procedure (e.g., Barnett et al., 2012; Neuman and Wierenga, 2002). Technical guidance manuals (e.g., Ohio EPA, 2007; Reilly and Harbaugh, 2004) describe general modeling procedures usually intended for a specific audience of modelers. The ASTM International (<http://www.astm.org/>) has published a variety of technical guidance documents on groundwater modeling (e.g., ASTM, 2006, 2008).

## 1.7 COMMON MODELING ERRORS

At the end of each chapter, we present modeling errors that we have found to be common mistakes and misconceptions in groundwater modeling. Because no such list can be inclusive, the reader will undoubtedly make modeling errors and encounter errors in the work of other modelers that are not included in our lists.

- The modeler does not allow enough time for calibration. Certainly formulation of the conceptual model and design of the numerical model are critical steps in groundwater modeling. However, modelers often spend so much time on those initial steps that they run out of time and budget for robust model calibration; we suggest that half of the project’s time and budget should be allocated for calibration.
- The modeler does not allow enough time for forecasting simulations. Modelers tend to think that the hard work of modeling is over when the model has been calibrated and assume that the forecasting simulations will be straightforward “production” runs. However, it is essential to perform an uncertainty analysis in conjunction with the forecast (Chapter 10) and uncertainty analysis may occupy more time than the modeler anticipates. Furthermore, sometimes surprises are encountered during the forecasting simulations that may require the modeler to revisit some of the earlier steps in the modeling workflow.
- The modeler does not allow enough time for report preparation. A readable and comprehensive modeling report is invaluable for reconstructing important modeling decisions and outcomes. A model is diminished without a good report to describe the model and its results.

## 1.8 USE OF THIS TEXT

Readers should be familiar with the basic principles of groundwater hydrology and basic concepts of groundwater modeling presented in standard hydrogeology textbooks such as Fitts (2013), Kresic (2007), Todd and Mays (2005), Schwartz and Zhang (2003), and

Fetter (2001). In Chapter 3, we review basic principles of FD and FE methods drawing on the elementary level text by Wang and Anderson (1982).

The problems following each chapter are intended to illustrate the main points of the chapter. Starting with Chapter 4, most of the problems require the use of an FD or FE code. Boxes amplify topics mentioned in the main text.

To supplement the material covered in the text, the reader is encouraged to consult the literature cited throughout the book as well as groundwater journals and modeling reports published by the US. Geological Survey and other governmental and regulatory groups. We have included links to many such resources on the companion Web site for this text (<http://appliedgwmodeling.elsevier.com>). The modeler can develop modeling intuition and hydrosense by studying the models described in journal papers and technical reports, starting with those cited in our book, and by the experience of developing and solving problems with models.

## 1.9 PROBLEMS

Problems for Chapter 1 are intended to introduce the modeling process and stimulate thinking about the level of modeling needed to address a stated modeling purpose.

**P1.1** List the type of groundwater model (i.e., forecasting or interpretive (engineering calculator, screening, or generic)) that would most likely be used to solve each of the following problems. List the assumptions you made to reach your decision.

- a. A regulatory agency wants to understand why the ages of water discharging from various springs that flow from an anisotropic and homogeneous sandstone aquifer are so variable. It is suggested that each spring is discharging water that is a mix of water coming from several different flowpaths, or that stratigraphic and structural controls affect groundwater residence times and thus determine the age of the spring discharge.
- b. A lawyer wants a consultant to estimate seasonal fluctuations in the water table of an alluvial fan aquifer in Spain resulting from a change in the timing and distribution of groundwater recharge originating from flood irrigation practices. The change in recharge was brought about by recent litigation involving land ownership.
- c. A consulting firm is tasked to determine the scales and magnitudes of aquifer heterogeneities that would cause a 25% reduction in the size of the capture zone of a well designed to pump contaminated water from what was thought to be a homogeneous unconfined outwash aquifer.
- d. A stream ecologist wants to quantify the seasonal exchange of water between a stream and its contiguous floodplain aquifer.
- e. An agency is planning a secure landfill for disposal of low-level nuclear waste in thick low permeability sedimentary deposits. The agency would like to assess



the effect of changes in recharge on rates and directions of groundwater flow at the proposed site.

- P1.2** Make a list of criteria you would use to determine if a model appropriately represented a particular hydrogeological system. Justify your selection and save the list for future reference.
- P1.3** Read a recent report prepared by a consultant or governmental agency that describes the application of a groundwater flow model in your geographical area. Identify the purpose of the model and the modeling question(s). How was the conceptual model presented (e.g., in text, cross sections, tables)? Describe the mathematical model and identify the code used to solve the model. Describe the calibration process. If the model was used for forecasting, discuss how the modeler(s) evaluated forecast uncertainty. Create a flow chart of the modeling process used and compare and contrast it to Fig. 1.1.

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